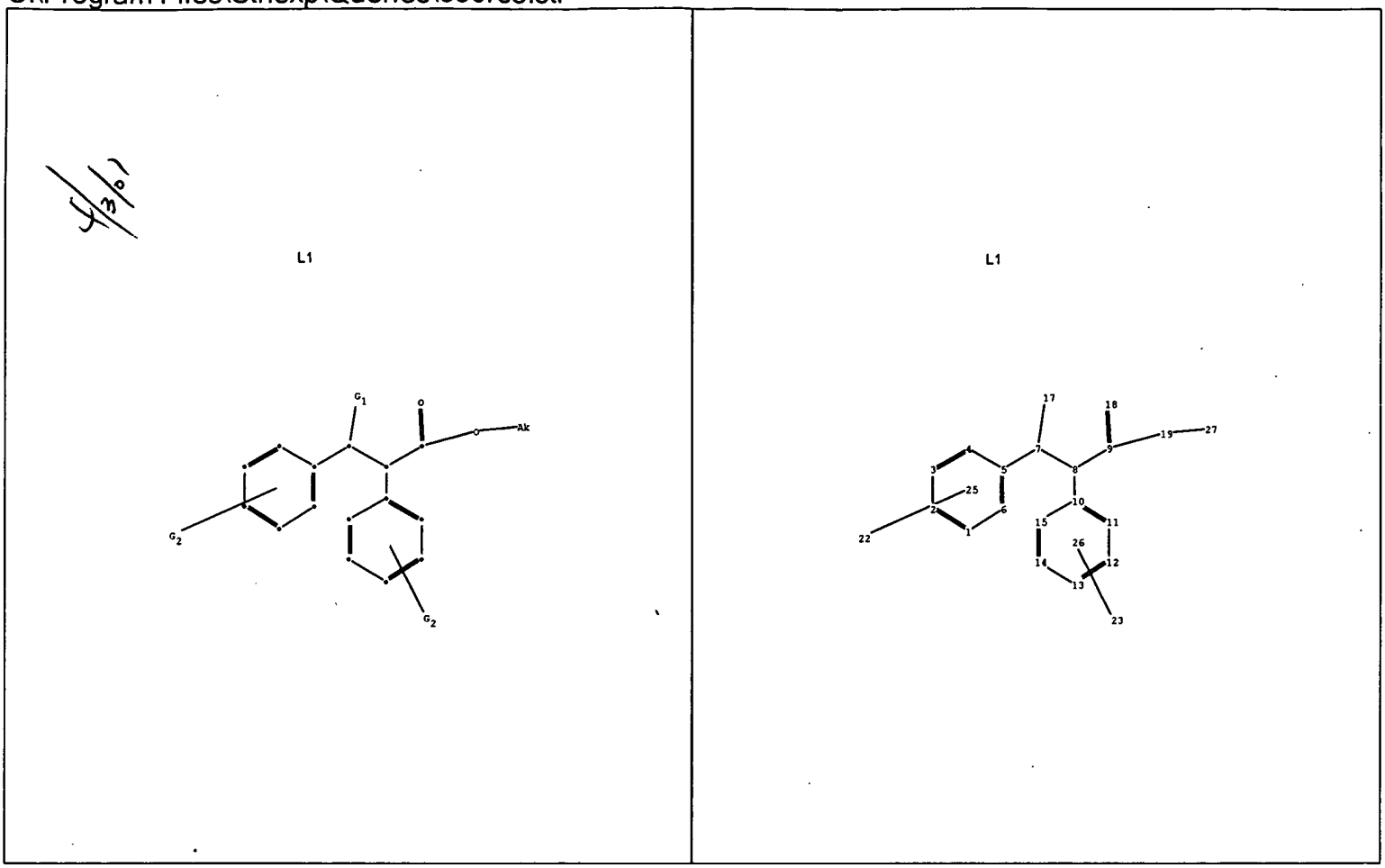
C:\Program Files\Stnexp\Queries\690rce.str



chain nodes :
7 8 9 17 18 19 22 23 27 29
ring nodes :
1 2 3 4 5 6 10 11 12 13 14 15
chain bonds :
5-7 7-8 7-17 8-9 8-10 9-18 9-19 19-27
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 10-11 10-15 11-12 12-13 13-14 14-15
exact/norm bonds :
7-17 9-18 9-19 19-27
exact bonds :
5-7 7-8 8-9 8-10
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 10-11 10-15 11-12 12-13 13-14 14-15

G1:CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu,OH,H

G2:CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,MeO,EtO,n-PrO,i-PrO,NH2,NO2

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 17:CLASS 18:CLASS 19:CLASS 22:CLASS 23:CLASS 25:Atom 26:Atom 27:CLASS

CAS ONLINE PRINTOUT

=> d his

(FILE 'REGISTRY' ENTERED AT 08:23:30 ON 03 APR 2007)
DELETE HIS
L1 STRUCTURE UPLOADED
L2 9 S L1
L3 217 S L1 FUL
L4 22 SEARCH L1 CSS SUB=L3 FULL

FILE 'CAPLUS' ENTERED AT 08:25:37 ON 03 APR 2007
L5 16 S L4

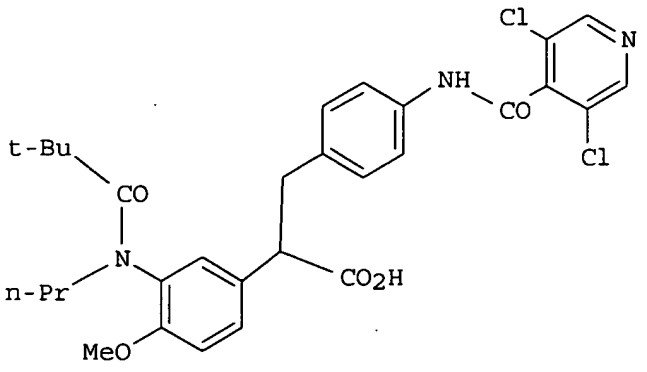
=> d l1
L1 HAS NO ANSWERS
L1 STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

=> d l5 bib abs hitstr 1-16

L5 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2004:1068280 CAPLUS
DN 142:126564
TI 2,3-Diphenylpropionic acids as potent VLA-4 antagonists
AU Hoshina, Yoichiro; Ikegami, Satoru; Okuyama, Akihiko; Fukui, Hideto; Inoguchi, Kiyoshi; Maruyama, Tatsuya; Fujimoto, Kyoko; Matsumura, Yuzuru; Aoyama, Akinori; Harada, Tatsuhiro; Tanaka, Hiroshi; Nakamura, Tsutomu
CS Central Research Laboratories, Ltd., Kaken Pharmaceutical Co., Yamashina, Kyoto, 607-8042, Japan
SO Bioorganic & Medicinal Chemistry Letters (2005), 15(1), 217-220
CODEN: BMCLE8; ISSN: 0960-894X
PB Elsevier B.V.
DT Journal
LA English
OS CASREACT 142:126564
GI



I

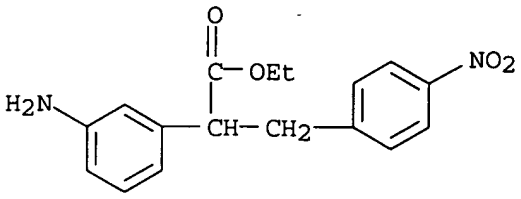
AB The discovery and SAR of 2,3-diphenylpropionic acid derivs. as highly

potent VLA-4 antagonists are described. One representative compound, I has inhibited intercellular adhesion by a VCAM-1/VLA-4 interaction with an IC50 of 1.7 nM, and has good pharmacokinetics and oral bioavailability.

IT 400648-51-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(2,3-Diphenylpropionic acids as potent VLA-4 antagonists)

RN 400648-51-3 CAPLUS

CN Benzenepropanoic acid, α-(3-aminophenyl)-4-nitro-, ethyl ester (9CI) (CA INDEX NAME)

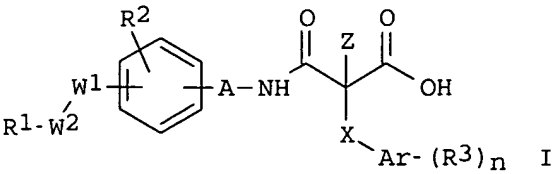


RE.CNT 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2004:931493 CAPLUS
DN 141:410707
TI Preparation of malonic acids as protein tyrosine phosphatase (PTP) inhibitors and their pharmaceutical use
IN Amanomiya, Yoshiya; Motoizumi, Masatoshi; Taniuchi, Makoto
PA Sankyo Co., Ltd., Japan
SO Jpn. Kokai Tokkyo Koho, 166 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 2004307460	A	20041104	JP 2003-198893	20030718
PRAI	JP 2002-212121	A	20020722		
	JP 2003-43056	A	20030220		

OS MARPAT 141:410707
GI

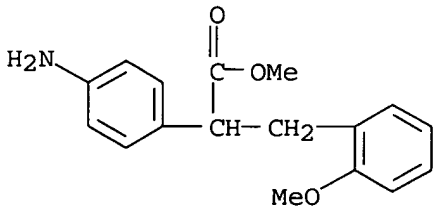


AB Title compds. I [Ar = C6-10 aromatic; A = bond, CH2, C1-3 oxyalkylene; W1 = bond, oxyalkylene CO, O, CONH; W2 = bond, C6H4, C6H4O, C6H4CO, CH2CO; X = O, CH2; Z = H, F; R1 = C5-20 linear alkyl, C7-20 linear alkenyl, C7-20 linear alkadienyl, (un)substituted piperazinyl, (un)substituted Ph, etc; R2 = H, OH, O(CH2)naCO2h (na = 1-6); R2W1 may form ring; R3 = H, C1-6 alkyl, (CO2H-substituted) C1-6 alkoxy, CO2H; n = 1-3], useful for treatment of diabetes, obesity, hyperlipidemia, allergy, etc., are prepared

Thus, amidation of 2-ethoxycarbonyl-3-phenylpropionic acid with 4-nitroaniline gave Et 2-(4-nitrophenylaminocarbonyl)-3-phenylpropionate, which was hydrogenated, amidated with palmitoyl chloride, and hydrolyzed to afford 2-[N-[4-(hexadecanoylamino)phenyl]aminocarbonyl]-3-phenylpropionic acid, which inhibited 92% human PTP-1B activity.

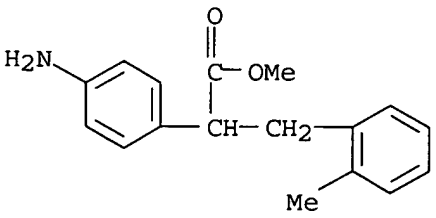
IT 790259-89-1P 790260-04-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of malonic acids as protein tyrosine phosphatase inhibitors for treatment of diseases)

RN 790259-89-1 CAPLUS
CN Benzenepropanoic acid, α-(4-aminophenyl)-2-methoxy-, methyl ester, hydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 790260-04-7 CAPLUS
CN Benzenepropanoic acid, α-(4-aminophenyl)-2-methyl-, methyl ester, hydrochloride (9CI) (CA INDEX NAME)

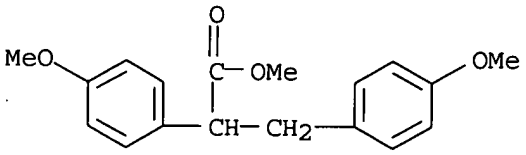


● HCl

L5 ANSWER 3 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2004:261264 CAPLUS
DN 141:399
TI Discovery of Diarylacrylonitriles as a Novel Series of Small Molecule Sortase A Inhibitors
AU Oh, Ki-Bong; Kim, Soo-Hwan; Lee, Jaekwang; Cho, Won-Jea; Lee, Taeho; Kim, Sanghee
CS Natural Products Research Institute, College of Pharmacy, Seoul National University, Seoul, 110-460, S. Korea
SO Journal of Medicinal Chemistry (2004), 47(10), 2418-2421
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal

CAS ONLINE PRINTOUT

LA English
OS CASREACT 141:399
AB On the basis of a hit from random screening, a novel class of small-mol. sortase A inhibitors was generated. The primary structure-activity relationship and the minimal structural requirements for potency were established through structural modifications and mol. modeling studies.
IT 380914-92-1
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(discovery of diarylacrylonitriles as a novel series of small mol. sortase A inhibitors)
RN 380914-92-1 CAPLUS
CN Benzenepropanoic acid, 4-methoxy-α-(4-methoxyphenyl)-, methyl ester (9CI) (CA INDEX NAME)

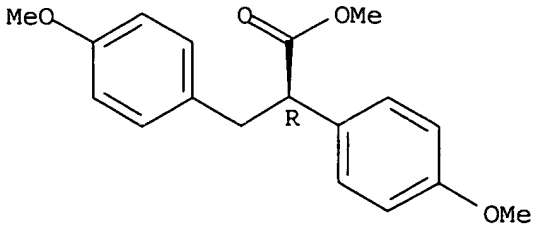


RE.CNT 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2003:262921 CAPLUS
DN 139:85155
TI Intermolecular C-H activation at benzylic positions: synthesis of (+)-imperanene and (-)-α-conidendrin
AU Davies, Huw M. L.; Jin, Qihui
CS Department of Chemistry, University at Buffalo, The State University of New York, Buffalo, NY, 14260-3000, USA
SO Tetrahedron: Asymmetry (2003), 14(7), 941-949
CODEN: TASYE3; ISSN: 0957-4166
PB Elsevier Science Ltd.
DT Journal
LA English
OS CASREACT 139:85155
AB An efficient C-H activation of primary benzylic positions by means of rhodium carbenoid induced C-H insertions is described. This key step was used in concise syntheses of (+)-imperanene and (-)-α-conidendrin.
IT 553642-25-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of (+)-imperanene and (-)-α-conidendrin from a benzene derivative and a aryldiazoacetate via a rhodium carbenoid induced C-H insertion)
RN 553642-25-4 CAPLUS
CN Benzenepropanoic acid, 4-methoxy-α-(4-methoxyphenyl)-, methyl ester, (αR)- (9CI) (CA INDEX NAME)

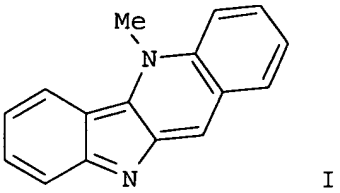
Absolute stereochemistry. Rotation (-).

CAS ONLINE PRINTOUT

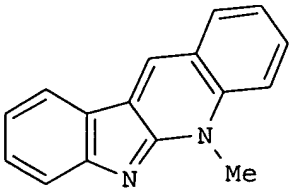


RE.CNT 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 5 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2003:4433 CAPLUS
DN 138:238326
TI Synthesis of cryptolepine and cryptoteckieine from a common intermediate
AU Ho, Tse-Lok; Jou, Der-Guey
CS Department of Applied Chemistry, National Chiao Tung University, Hsinchu, Taiwan
SO Helvetica Chimica Acta (2002), 85(11), 3823-3827
CODEN: HCACAV; ISSN: 0018-019X
PB Verlag Helvetica Chimica Acta
DT Journal
LA English
OS CASREACT 138:238326
GI



I

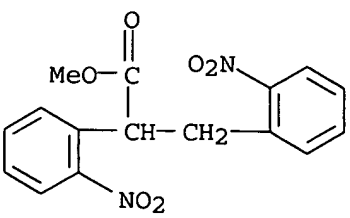


II

AB Both cryptolepine I and cryptoteckieine II have been synthesized from 1,3-bis(2-nitrophenyl)propan-2-one. The approach to I involved reduction of the NO2 groups, oxidative cyclization with PhI(OAc)2, and N-methylation, whereas II was obtained via bromination, Favorskii rearrangement, reduction (in situ cyclization), and N-methylation.

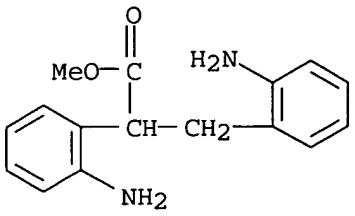
IT 500904-96-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of cryptolepine and cryptoteckieine from 1,3-bis(2-nitrophenyl)propan-2-one)

RN 500904-96-1 CAPLUS
CN Benzenepropanoic acid, 2-nitro-α-(2-nitrophenyl)-, methyl ester (9CI) (CA INDEX NAME)



CAS ONLINE PRINTOUT

IT 500904-98-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of cryptolepine and cryptoteckieine from 1,3-bis(2-nitrophenyl)propan-2-one)
RN 500904-98-3 CAPLUS
CN Benzenepropanoic acid, 2-amino-α-(2-aminophenyl)-, methyl ester (9CI) (CA INDEX NAME)



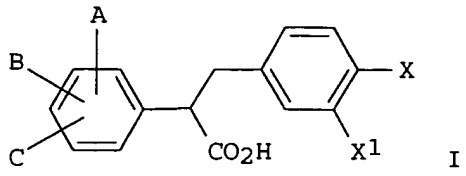
RE.CNT 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 6 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2002:142657 CAPLUS
DN 136:183822
TI Preparation of 2,3-diphenylpropionic acid derivatives or their salts, medicines or cell adhesion inhibitors containing the same, and their usage
IN Hoshina, Yoichiro; Ikegami, Satoru; Matsuo, Atsushi; Harada, Tatsuhiro; Okuyama, Akihiko
PA Kaken Pharmaceutical Co., Ltd., Japan
SO PCT Int. Appl., 162 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002014262	A1	20020221	WO 2001-JP6934	20010810
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU 2001078709	A5	20020225	AU 2001-78709	20010810
	CA 2419008	A1	20030211	CA 2001-2419008	20010810
	EP 1325903	A1	20030709	EP 2001-956840	20010810
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	US 2004072878	A1	20040415	US 2003-344105	20030819
PRAI	JP 2000-244226	A	20000811		
	JP 2001-115840	A	20010413		
	WO 2001-JP6934	W	20010810		

OS MARPAT 136:183822
GI

CAS ONLINE PRINTOUT



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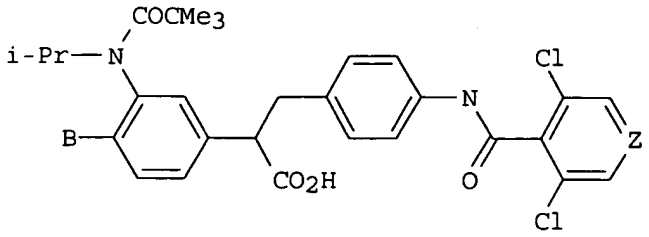


II

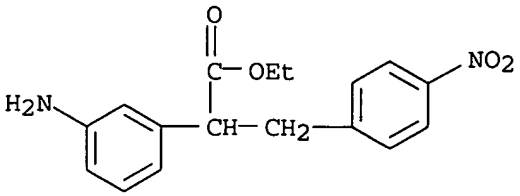
AB The title compds. [I; A, B, C = H, halo, NO2, cyano, OH, CO2H, alkyl, aryl, heteroaryl, alkoxy, aryloxy, heteroaryloxy, alkyloxycarbonyl, aryloxycarbonyl, heteroaryloxycarbonyl, alkanoyl, aroyl, heteroaroyl, alkylcarbonyloxy, arylcarbonyloxy, heteroarylcarbonyloxy, alkylthio, arylthio, heteroarylthio, alkylthio, arylthio, heteroarylthio, alkylsulfonyl, arylsulfonyl, heteroarylsulfonyl, alkylsulfinyl, arylsulfinyl, heteoarylsulfinyl, NR1R2, NR1COR2, NR1SO2R2, NR1CONR2R3, CONR1R2 (wherein R1, R2, R3 = H, alkyl, alkenyl, alkoxy, aryl, aryloxy, heteroaryloxy, or heteroaryl, or R1 and R2 or R2 and R3 are linked to each other to form a (un)substituted ring optionally containing at least one ring atom selected from O, N, and S and optionally containing a double bond); or when two of A, B, and C are linked to adjacent carbon atoms, they form a benzene ring or methylenedioxy; X, X1 = H, halo, NO2, cyano, OH, CO2H, alkyl, alkenyl or alkynyl, aryl, heteroaryl, alkoxy, aryloxy, heteroaryloxy, alkanoyl, aroyl, heteroaroyl, alkylcarbonyloxy, arylcarbonyloxy, heteroarylcarbonyloxy, alkylthio, arylthio, heteroarylthio, heteroaryloxycarbonyl, alkylthio, arylthio, heteroarylthio, alkylsulfonyl, arylsulfonyl, heteroarylsulfonyl, alkylsulfinyl, arylsulfinyl, heteoarylsulfinyl, NR4R5, NR4COR5, NR4SO2R5, NR4CONR5R6, O2CNR4R5, CONR4R5 (where R4 - R6 group listed in R1 - R3)] or their salts are prepared Also claimed are cell adhesion inhibitors, integrin VLA-4 (α4β1) and/or LPAM-1 (α4β7) antagonists, α4 integrin inhibitors, or therapeutics or preventives inflammatory diseases related to cell adhesion process containing I or the salts as the active ingredients. These compds. are superior in oral absorption and in vivo dynamic. Thus, acylation of 3-(4-aminophenyl)-2-[3-[(2,2-dimethylpropionyl)isobutylamino]-4-methoxyphenyl]propionic acid Et ester by 2,6-dichlorobenzoyl chloride in pyridine gave 71% 3-[4-(2,6-dichlorobenzoylamino)phenyl]-2-[3-[(2,2-dimethylpropionyl)isobutylamino]-4-methoxyphenyl]propionic acid Et ester which was saponified with a mixture of aqueous NaOH, THF, and MeOH followed by acidification with aqueous HCl to give 91% 2,3-diphenylpropionic acid derivative (II; B = MeO, Z = CH) (III). III and II (B = Et, Z = N) inhibited adhesion of myeloid leukemic cells HL-60 expressing VLA-4 to Chinese hamster (CHO) cells expressing human VCAM-1 with IC50 of 2 and 0.1 nM, resp.

IT 400648-51-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 2,3-diphenylpropionic acid derivs. or their salts as cell adhesion inhibitors, integrin antagonists or inhibitors, and antiinflammatory agents)

RN 400648-51-3 CAPLUS

CAS ONLINE PRINTOUT

CN Benzenepropanoic acid, α-(3-aminophenyl)-4-nitro-, ethyl ester (9CI) (CA INDEX NAME)



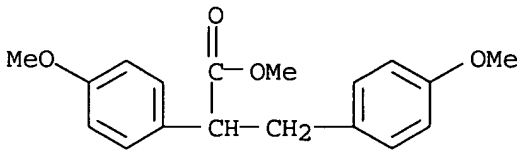
RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 7 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2001:752301 CAPLUS
DN 136:47979
TI Estrogen Receptor-β Potency-Selective Ligands: Structure-Activity Relationship Studies of Diarylpropionitriles and Their Acetylene and Polar Analogues
AU Meyers, Marvin J.; Sun, Jun; Carlson, Kathryn E.; Marriner, Gwendolyn A.; Katzenellenbogen, Benita S.; Katzenellenbogen, John A.
CS Departments of Chemistry Molecular and Integrative Physiology and Cell and Structural Biology, University of Illinois, Urbana, IL, 61801, USA
SO Journal of Medicinal Chemistry (2001), 44(24), 4230-4251
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
OS CASREACT 136:47979
AB Through an effort to develop novel ligands that have subtype selectivity for the estrogen receptors alpha (ERα) and beta (ERβ), we have found that 2,3-bis(4-hydroxyphenyl)propionitrile (DPN) acts as an agonist on both ER subtypes, but has a 70-fold higher relative binding affinity and 170-fold higher relative potency in transcription assays with ERβ than with ERα. To investigate the ERβ affinity- and potency-selective character of this DPN further, we prepared a series of DPN analogs in which both the ligand core and the aromatic rings were modified by the repositioning of phenolic hydroxy groups and by the addition of alkyl substituents and nitrile groups. We also prepared other series of DPN analogs in which the nitrile functionality was replaced with acetylene groups or polar functions, to mimic the linear geometry or polarity of the nitrile, resp. To varying degrees, all of the analogs show preferential binding affinity for ERβ (i.e., they are ERβ affinity-selective), and many, but not all of them, are also more potent in activating transcription through ERβ than through ERα (i.e., they are ERβ potency-selective). meso-2,3-Bis(4-hydroxyphenyl)succinonitrile and dl-2,3-bis(4-hydroxyphenyl)succinonitrile are among the highest ERβ affinity-selective ligands, and they have an ERβ potency selectivity that is equivalent to that of DPN. The acetylene analogs have higher binding affinities but somewhat lower selectivities than their nitrile counterparts. The polar analogs have lower affinities, and only the fluorinated polar analogs have substantial affinity selectivities. This study suggests that, in this series of ligands, the nitrile functionality is critical to ERβ selectivity because it provides the optimal combination of linear geometry and polarity. Furthermore, the addition of a second nitrile group β to the nitrile in DPN or the addition of a Me substituent at an ortho position on the β-aromatic ring increases the affinity and selectivity of these

compds. for ERβ. These ERβ-selective compds. may prove to be valuable tools in understanding the differences in structure and biol. function of ERα and ERβ.

IT 380914-92-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and structure activity relations of diarylpropionitriles and their acetylene and polar analogs as estrogen receptor-β selective ligands)

RN 380914-92-1 CAPLUS
CN Benzenepropanoic acid, 4-methoxy-α-(4-methoxyphenyl)-, methyl ester (9CI) (CA INDEX NAME)



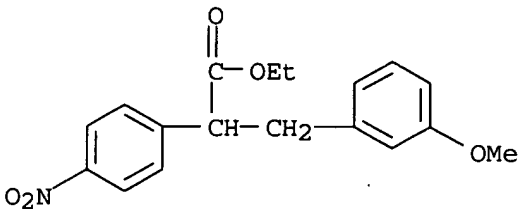
RE.CNT 72 THERE ARE 72 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 8 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1999:436718 CAPLUS
DN 131:184605
TI Intramolecular cyclizations via arylnitrenium ions. Formation of a six-membered ring rather than a macrocycle
AU Abramovitch, Rudolph A.; Ye, Xiaocong
CS Department of Chemistry, Clemson University, Clemson, SC, 29634-1905, USA
SO Journal of Organic Chemistry (1999), 64(16), 5904-5912
CODEN: JOCEAH; ISSN: 0022-3263
PB American Chemical Society
DT Journal
LA English
AB The stereochem. of 1-(3-benzyloxyphenyl)-2-(4-nitrophenyl)ethane has been studied. MMX calcns. predicted, and 2D NOESY confirmed, that the bent conformation (global energy min.) was such that six-membered ring formation, and not macrocyclization, would occur using the corresponding nitrenium ion, and this was found to be the case. Acid-catalyzed decomposition of 1-(3-benzyloxyphenyl)-2-(4-azidophenyl)ethane followed by treatment with (CF3CO)2O gave 48% of 2-benzyloxy-6-trifluoroacetamido-9,10-dihydrophenanthrene and 18% of 1-(3-benzyloxyphenyl)-2-(4-trifluoroacetamidophenyl)ethane. Blocking the original point of attack with a bromine atom led to the prediction (MMX, 2D NOESY) that, once again, small ring formation would take place, with macrocyclization possible but less likely. Again, this was found to be so. It is suggested that simple MMX calcns. may provide a very rapid, empirical indicator of which precursors would have a readily accessible conformation that could result in intramol. cyclization leading to macrocycles being preferred over intermol. reactions.

IT 239445-37-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(hydrolysis of; exptl. and mol. mechanics MMX-based conformational prediction of six-membered ring formation vs. macrocyclization in intramol. cyclization reactions involving arylnitrenium ions)

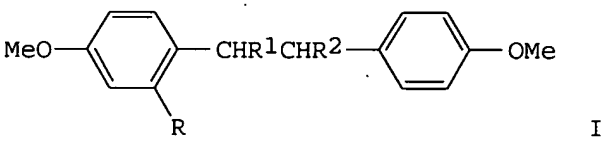
RN 239445-37-5 CAPLUS
CN Benzenepropanoic acid, 3-methoxy-α-(4-nitrophenyl)-, ethyl ester (9CI) (CA INDEX NAME)

CAS ONLINE PRINTOUT



RE.CNT 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 9 OF 16 CAPLUS . COPYRIGHT 2007 ACS on STN
AN 1984:138677 CAPLUS
DN 100:138677
TI Silicon-mediated synthesis of bibenzyl systems: synthesis of ring and side-chain functionalized hexestrol derivatives
AU Mohan, Raju; Katzenellenbogen, John A.
CS Sch. Chem. Sci., Univ. Illinois, Urbana, IL, 61801, USA
SO Journal of Organic Chemistry (1984), 49(7), 1238-46
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
OS CASREACT 100:138677
GI

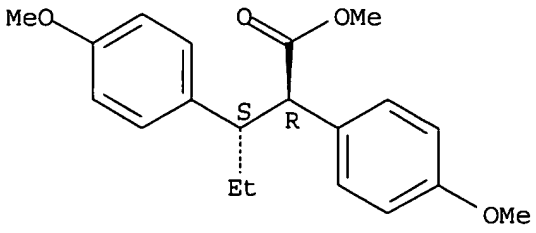


I

AB Hexestrol derivs. I (R = H, NO2; R1 = CH:CH2, R2 = Me, Et) were prepared by benzylic coupling of alkylsilanes 2,4-R(MeO)C6H3CH:CHCH2SiMe3 (II) with 4-R3C6H4OMe (R3 = CHEtOMe, CHEtCl, CHMeOMe). The allylsilanes were prepared from 2,4-R(MeO)C6H3CHO (III; R = H, NO2) and Ph3P:CHCH2SiMe3 (IV). III (R = Me3Si) reacted similarly with IV to give II. Diastereomeric I (R = H, NO2; R1 = CH:CH2; R2 = Me, Et) were readily separated, and hydrogenation of I (R = NO2, R1 = CH:CH2, R2 = Me, Et) gave I (R1 = Et). 4-MeOC6H4CH2CO2Me was silylated and treated with 4-MeOC6H4CHClEt to give diastereomeric I (R = H, R1 = Et, R2 = CO2Me). This method. represents a convenient synthetic route to hexestrol and norhexestrol derivs.
IT 83303-94-0P 88932-62-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 83303-94-0 CAPLUS
CN Benzenepropanoic acid, β-ethyl-4-methoxy-α-(4-methoxyphenyl)-, methyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

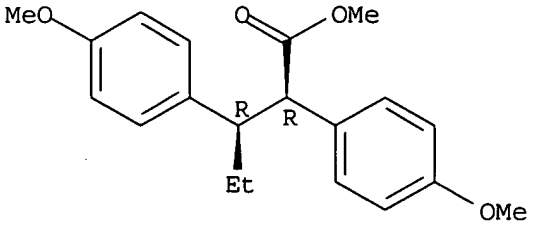
Relative stereochemistry.

CAS ONLINE PRINTOUT



RN 88932-62-1 CAPLUS
CN Benzenepropanoic acid, β-ethyl-4-methoxy-α-(4-methoxyphenyl)-, methyl ester, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

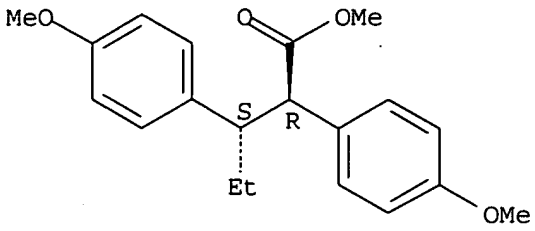


L5 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1982:582080 CAPLUS
DN 97:182080
TI Nonsteroidal estrogens: synthesis and estrogen receptor binding affinity of derivatives of (3R*,4S*)-3,4-bis(4-hydroxyphenyl)hexane (hexestrol) and (2R*,3S*)-2,3-bis(4-hydroxyphenyl)pentane (norhexestrol) functionalized on the side chain
AU Landvatter, Scott W.; Katzenellenbogen, J. A.
CS Sch. Chem. Sci., Univ. Illinois, Urbana, IL, 61801, USA
SO Journal of Medicinal Chemistry (1982), 25(11), 1300-7
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
OS CASREACT 97:182080
AB A series of nonsteroidal, side-chain-functionalized estrogens based on (3R*,4S*)-3,4-bis(4-hydroxyphenyl)hexane (hexestrol) and (2R*,3S*)-2,3-bis(4-hydroxyphenyl)pentane (norhexestrol) were prepared and included amide, diazo ketone, ester, alc., ketone, fluoro, bromo, iodo, and saturated hydrocarbon derivs. Thus, Me (2R*,3S*)-2,3-bis(4-methoxyphenyl)pentanoate was treated with BBr3 and NH3 to give (2R*,3S*)-2,3-bis(4-hydroxyphenyl)pentanamide. Anal. of the binding affinity of these compds. to the uterine estrogen receptor, measured by competitive binding assay, reveals trends that can be related to the steric size, the hydrophobicity, and the hydrogen bond accepting character of the side-chain substituents. Comparison of binding affinities between norhexestrol and hexestrol derivs. indicates that, in general, the norhexestrols show significantly higher receptor binding affinities, making this series of compds. ideally suited as functional probes for the estrogen receptor.
IT 83303-94-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(amidation of)
RN 83303-94-0 CAPLUS
CN Benzenepropanoic acid, β-ethyl-4-methoxy-α-(4-methoxyphenyl)-,

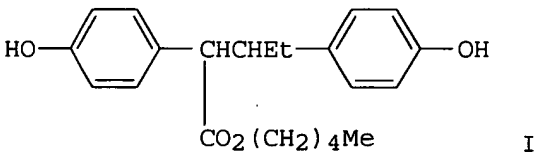
CAS ONLINE PRINTOUT

methyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L5 ANSWER 11 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1981:615317 CAPLUS
DN 95:215317
TI Stereochemical considerations in the binding of nonsteroidal estrogens to the estrogen receptor
AU Landvatter, Scott W.; Katzenellenbogen, John A.
CS Sch. Chem. Sci., Univ. Illinois, Urbana, IL, 61801, USA
SO Molecular Pharmacology (1981), 20(1), 43-51
CODEN: MOPMA3; ISSN: 0026-895X
DT Journal
LA English
GI



I

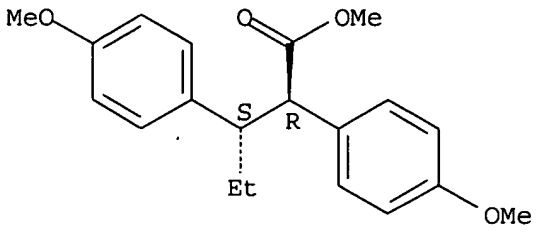
AB Derivs. of nonsteroidal estrogens, such as hexestrol, can interact with the estrogen receptor in 4 possible binding modes, 2 per enantiomer. Several side chain-functionalized hexestrol and norhexestrol derivs. have been synthesized and resolved into pure enantiomers. Binding studies with lamb uterine estrogen receptor have indicated that there is no appreciable difference in binding between enantiomers in the hexestrol series. Enantiomers in the norhexestrol series, on the other hand, do show differences in binding. The (-)-(2R,3S)-pentyl ester (I) [79568-12-0] binds to receptor with twice the affinity of racemic material and 14 times the affinity of the (+)-(2S,3R)-antipode [78923-77-0]. It is concluded that the norhexestrols prefer 1 of the 4 possible binding modes, whereas the hexestrols can adopt 2 of the 4 modes equally. Furthermore, comparisons between the binding affinities of corresponding hexestrol and norhexestrol derivs. suggest that the source of chiral recognition is a specific interaction between the carbonyl group in the 2R,3S enantiomer of the norhexestrol derivs. that elevates affinity, this interaction not being attainable in the other enantiomer and in the derivs. in the hexestrol series.

IT 83303-94-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and estrogen receptor binding of)
RN 83303-94-0 CAPLUS

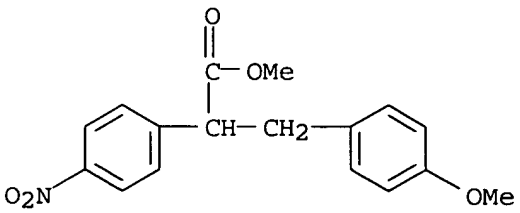
CAS ONLINE PRINTOUT

CN Benzenepropanoic acid, β-ethyl-4-methoxy-α-(4-methoxyphenyl)-, methyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L5 ANSWER 12 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1974:107684 CAPLUS
DN 80:107684
TI Complex metal hydride reduction of carbon-carbon unsaturation. I. Sodium borohydride reduction of α-phenylcinnamates and related systems
AU Schauble, J. Herman; Walter, Gerald J.; Morin, J. Guy
CS USA
SO Journal of Organic Chemistry (1974), 39(6), 755-60
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
AB Competitive rates of NaBH4 reduction for two sets of Me α-phenyl-trans-cinnamates, para-substituted in the α and β rings, resp., correlate linearly with Hammett substituent consts. The similarity in ρα (1.74) and ρβ (1.44) indicates that the transition state for hydride transfer occurs before significant change in geometry of the α,β-unsatd. carbonyl system occurs. Competitive rate studies for Me α-(para-substituted phenyl)acrylates and Me α-phenyl-cis- and -trans-crotonates are corroborated by the data obtained for the cinnamates.
IT 50415-54-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 50415-54-8 CAPLUS
CN Benzenepropanoic acid, 4-methoxy-α-(4-nitrophenyl)-, methyl ester (9CI) (CA INDEX NAME)

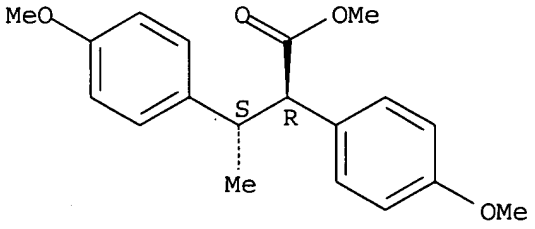


L5 ANSWER 13 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1970:465913 CAPLUS
DN 73:65913
TI Antiestrogenic and antifertility compounds. III. Enantiomers of (+-)-hexestrol and its homologs
AU Collins, Dennis J.; Hobbs, John J.
CS Dep. Vet. Physiol., Univ. Sydney, Sydney, Australia

CAS ONLINE PRINTOUT

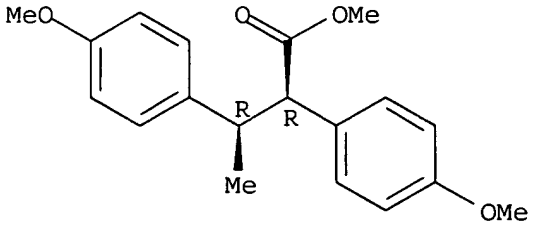
SO Australian Journal of Chemistry (1970), 23(8), 1605-24
CODEN: AJCHAS; ISSN: 0004-9425
DT Journal
LA English
AB (±)-2,3-Bis(p-hydroxyphenyl)butane (I) and (±)-3,4-bis(p-hydroxyphenyl)hexane were resolved, and the absolute stereochemistry of I was determined as (-)-(2R,3R) by correlation with (+)-(R)-2,3-bis(p-methoxyphenyl)-1-butene. (+)- and (-)-erythro-2,3-Bis(p-hydroxyphenyl)pentane (-)-erythro-II% were synthesized from (-)- and (+)-erythro-2,3-bis(p-methoxyphenyl)valeric acid, resp. (+)-erythro-II is (2R,3S) and (+)-threo-(II) is (2S,3S) (correlation with (-)-(S)-2,3-bis(p-methoxyphenyl)-1-pentene). Thus, erythro-2,3-bis(p-methoxyphenyl)valeric and -butyric acids are (+)-(2S,3R). Interaction of optically active hexestrol and its homologs with the estrogen receptor site is discussed in terms of steroid stereochemistry.
IT 29550-19-4P 29550-20-7P 29551-32-4P
29551-42-6P 29555-63-3P 29555-64-4P
29555-67-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 29550-19-4 CAPLUS
CN Butyric acid, 2,3-bis(p-methoxyphenyl)-, methyl ester, erythro- (8CI) (CA INDEX NAME)

Relative stereochemistry.



RN 29550-20-7 CAPLUS
CN Butyric acid, 2,3-bis(p-methoxyphenyl)-, methyl ester, threo- (8CI) (CA INDEX NAME)

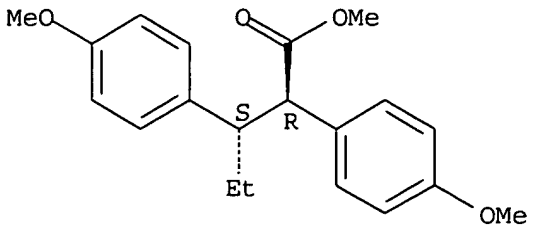
Relative stereochemistry.



RN 29551-32-4 CAPLUS
CN Benzenepropanoic acid, β-ethyl-4-methoxy-α-(4-methoxyphenyl)-, methyl ester, (R*,S*)-(+)- (9CI) (CA INDEX NAME)

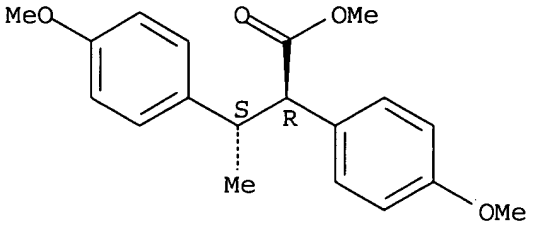
Rotation (+). Absolute stereochemistry unknown.

CAS ONLINE PRINTOUT



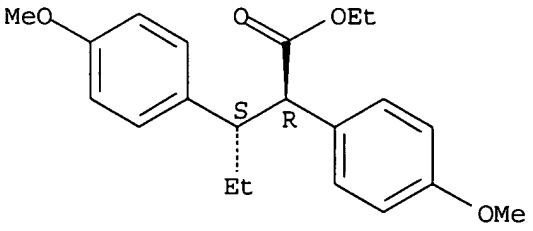
RN 29551-42-6 CAPLUS
CN Butyric acid, 2,3-bis(p-methoxyphenyl)-, methyl ester, erythro-(+)- (8CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.



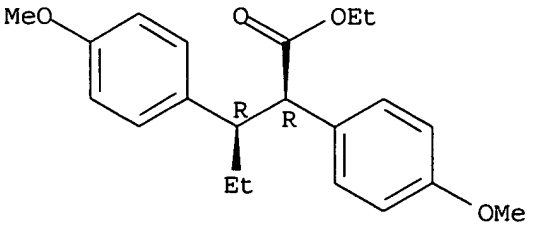
RN 29555-63-3 CAPLUS
CN Valeric acid, 2,3-bis(p-methoxyphenyl)-, ethyl ester, erythro- (8CI) (CA INDEX NAME)

Relative stereochemistry.



RN 29555-64-4 CAPLUS
CN Valeric acid, 2,3-bis(p-methoxyphenyl)-, ethyl ester, threo- (8CI) (CA INDEX NAME)

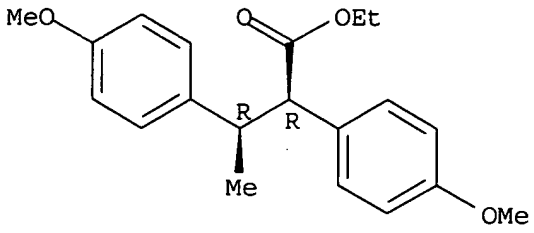
Relative stereochemistry.



RN 29555-67-7 CAPLUS
CN Butyric acid, 2,3-bis(p-methoxyphenyl)-, ethyl ester, erythro- (8CI) (CA INDEX NAME)

CAS ONLINE PRINTOUT

Relative stereochemistry.



L5 ANSWER 14 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1950:25021 CAPLUS
DN 44:25021
OREF 44:4932c-f
TI Synthetic estrogen
IN Hunter, James H.; Korman, Jerome
PA Upjohn Co.
DT Patent
LA Unavailable
FAN.CNT 1

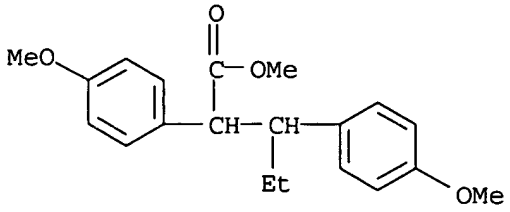
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2499920		19500307	US 1948-24413	19480430

AB 4,4'-Dimethoxy-α-cyanostilbene treated with EtMgBr yielded α,β-bis(p-methoxyphenyl) valeronitrile, which was saponified, esterified, demethylated, and reesterified to give α-methyl-α,β-bis(p-hydroxyphenyl)valeric acid (I), estrogenically active. EtMgBr from Mg 4.68 g. and EtBr 26.5 g. in anhydrous Et2O 200 ml. was added in small portions to 4,4'-dimethoxy-α-cyanostilbene 26.5 g., the mixture refluxed 24 hrs., cooled, decomposed with ice and dilute AcOH, and the Et2O layer washed with saturated NaHCO3 solution and water, dried over Na2SO4, and concentrated to give α,β-bis(p-methoxyphenyl)valeronitrile, m. 130-1°. This nitrile 12.1 g. with NaOH 4 g., water 8 ml., and (CH2OH)2 75 ml. was refluxed 36 hrs., water 90 ml. added, the mixture filtered hot, and the filtrate acidified when cool to yield a mixture of isomeric α,β-bis(p-methoxyphenyl)valeric acids, m. 177.5-9°. CH2N2 gave the corresponding Me ester, m. 128.5-30°. The ester (5 g.) in dry Et2O 50 ml. was mixed with 0.00178 mole Ph3CNa in Et2O 110 ml., and after 3 hrs. at room temperature, MeI 10 ml. added, the mixture let stand overnight, water and a few drops of AcOH added, the Et2O layer separated, and the crude product refluxed 22 hrs. with KOH 10 g. in 95% EtOH 150 ml., cooled, and acidified to obtain 4 g. of the mixed isomeric α-methyl-α,β-bis-(p-methoxyphenyl)valeric acids, m. 165-75°. Recrystn. gave 2.24 g. of the acid, m. 181-2.5°. The recrystd. acid (1 g.) and C5H5N.HCl 25 g. were heated at 185-95° 3 hrs., cooled, taken up in water, extracted with Et2O, and the Et2O washed with dilute HCl and water, dried, and concentrated to give I.

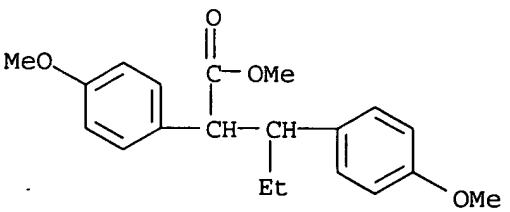
IT 857976-06-8P, Valeric acid, 2,3-bis(p-methoxyphenyl)-, methyl ester
RL: PREP (Preparation)
(preparation of)

RN 857976-06-8 CAPLUS
CN Valeric acid, 2,3-bis(p-methoxyphenyl)-, Me ester (5CI) (CA INDEX NAME)

CAS ONLINE PRINTOUT

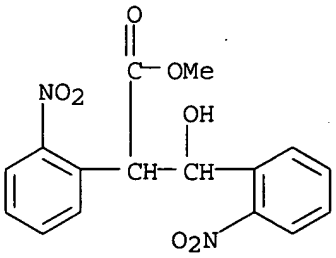


L5 ANSWER 15 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1949:2616 CAPLUS
DN 43:2616
OREF 43:613d-g
TI α-Methyl-α,β-bis(p-hydroxyphenyl)valeric acid, an active estrogen
AU Hunter, James H.; Korman, Jerome
SO Journal of the American Chemical Society (1948), 70, 3424-6
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA Unavailable
AB cf. C.A. 42, 160g. 4-MeOC6H4CH:C(CN)C6H4OMe-p (26.5 g.), added in small portions to EtMgBr (21.8 g. EtBr) in boiling ether, the mixture refluxed 24 hrs., and the red viscous oil crystallized from 95% EtOH, gives 10 g. α,β-bis(p-methoxyphenyl)-valeronitrile (I), m. 130-1°, and 13 g. of the isomer (II), yellow viscous oil, b0.03 220-30° (bath temperature). I (12.1 g.), 4 g. NaOH, 8 ml. H2O, and 75 ml. (CH2OH)2, refluxed 36 hrs., give a mixture of α,β-bis(p-methoxyphenyl)valeric acids which, crystallized from 95% EtOH, yields 4.65 g. of the isomer (III), m. 177.5-9°; II or a mixture of I and II yields the same acid; the residue (6 g.) from the alc. mother liquor, treated with CH2N2 in ether and the product crystallized from 95% EtOH, gives 4.92 g. of the Me ester, m. 93-4.5°, of the isomer (IV), m. 163-4.5°. The Me ester (V) of III m. 128.5-30°. V (5 g.) in 50 ml. ether, treated with 110 ml. of ethereal Ph3CNa (0.000162 mole/ml.) in a N atmospheric and, after 3 hrs. at room temperature, with 10 ml. MeI, the mixture kept overnight, and the residue refluxed 22 hrs. with 10 g. KOH in 150 ml. 95% EtOH, gives (on crystallization from BuOH) 2.24 g. α-methyl-α,β-bis(p-methoxyphenyl)-valeric acid (VI), m. 181-2.5°, and 0.07 g. of material m. 154-6°. VI (1 g.) and 25 g. C5H5N.HCl, heated 3 hrs. at 185-95°, give 0.8 g. α-methyl-α,β-bis(p-hydroxyphenyl)-valeric acid (VII), m. 225° (decomposition). VI is inactive in doses up to 500 γ, whereas VII produces the full estrus response in doses of 20 γ. Various unsuccessful attempts to prepare VII are recorded.
IT 857976-06-8P, Valeric acid, 2,3-bis(p-methoxyphenyl)-, Me ester
RL: PREP (Preparation)
(preparation of)
RN 857976-06-8 CAPLUS
CN Valeric acid, 2,3-bis(p-methoxyphenyl)-, Me ester (5CI) (CA INDEX NAME)



CAS ONLINE PRINTOUT

L5 ANSWER 16 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1927:18322 CAPLUS
DN 21:18322
OREF 21:2259h-i,2260a-b
TI Condensation of o-nitrophenylacetic acid with o-nitrobenzaldehyde
AU Kishi, N.
SO Yakugaku Zasshi (1926), No. 532, 475-81
CODEN: YKKZAJ; ISSN: 0031-6903
DT Journal
LA Unavailable
GI For diagram(s), see printed CA Issue.
AB By heating 4 g. o-o2NC6H4CH2CO2Na, 6 g o-O2NC2H4CHO and 30 g. Ac2O 5 hrs. at 140°, K. obtained a crystalline compound m. 244°(I). As far as the color reaction with H2SO4 is concerned I is similar to the stilbene compound obtained by Pschorr (Ber. 29,497(1896)), from the same compds. in the presence of ZnCl2; but its m. p. and composition are different. The analysis shows it has the compn.C15H12N2O7 and is α,β-di-o-nitrophenyl-β-hydroxypropionic acid. If this analysis is correct, the presence of OH is of unusual interest, since, in most aromatic condensations, OH is not retained. In spite of the fact that I cannot be benzoylated, nor acetylated by the usual method, a MeO derivative can be prepared by the action of MeI, showing that the OH group probably becomes more acid in nature, resisting replacement of the H by an acid group, in consequence of the presence of an o-nitro group. The MeO derivative m. 237°, and its Me ester m. 70°. The Me ester of I m. 74°. The OH group of I is very stable even at 160°, and does not change on boiling with concentrated HCl. When boiled with 10% KOH, it goes over to a compound m. 196°. When I is reduced with NH3-FeSO4, α,β-di[aminophenyl]-β-hydroxypropionic acid, m. 158°, is formed. HCl salt, decomps. 300°; when it is diazotized, and N is eliminated by Cu, a compound, m. 181° is formed, which is 8-amino-10-hydroxydihydrophenanthrene-9-carboxylic anhydride,
IT 872269-69-7P, Hydracrylic acid, α,β-bis(o-nitrophenyl)-, methyl ester
RL: PREP (Preparation)
(preparation of)
RN 872269-69-7 CAPLUS
CN Hydracrylic acid, α,β-bis(o-nitrophenyl)-, methyl ester (3CI) (CA INDEX NAME)



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